Predictions from the equation of state of cerium yield interesting insights into experimental results

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Outline

- A discussion of the model used and the differences of its approach
- Experimental results from front surface impact shots
- Phase diagram implications from the model
- Conclusions and suggested directions for the improvement of the model

Standard Helmholtz construction for each individual phase (α, γ, ε, liquid phases represented)

- **The Helmholtz energy is written as the following:**

$$F(V,T) = F_C(V) + F_H(V,T) + F_{AE}(V,T) - S_{tr}T$$

- **The cold curve energy function, F_c is given by the Vinet equation of state†**
- **F_H is described with the Debye approximation**
- **F_{AE} accounts for anharmonic lattice oscillations and electronic contributions is expressed as:**

$$F_{AE} = -\frac{1}{2} D \left(\frac{V}{V_{0K}} \right)^{\Gamma_{AE}} T^2$$

†Vinet, et. al., J. Phys.-Condensed Matter, **1**, 1941 (1989).

To describe the γ−α phase region the Aptekar-Ponyatovsky model was applied

- **The γ−α phases are modeled as a solid solution of both phases.**
- **The Gibbs energy function for the mixture is represented with the following equation:**

$$G = (1-c)G_{\alpha} + cG_{\gamma} + c(1-c)G_{mix} + TR(c\ln c + (1-c)\ln(1-c))$$

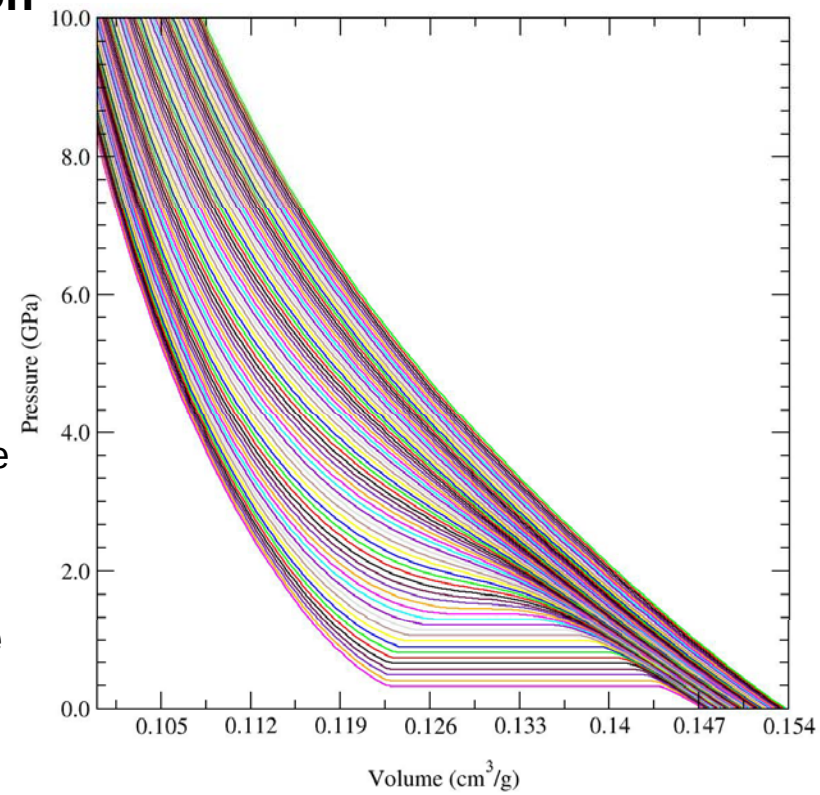
- **The G_{mix} term was said to be only a function of temperature**

$$G_{mix} = G_{mix}^{0}\left[1 + \frac{\theta_1}{T} + \left(\frac{\theta_2}{T}\right)^2\right]$$

- **Evaluating the partial derivative of *G* with respect to concentration and setting that quantity equal to zero allows one to determine the relative concentrations of each individual phase.**

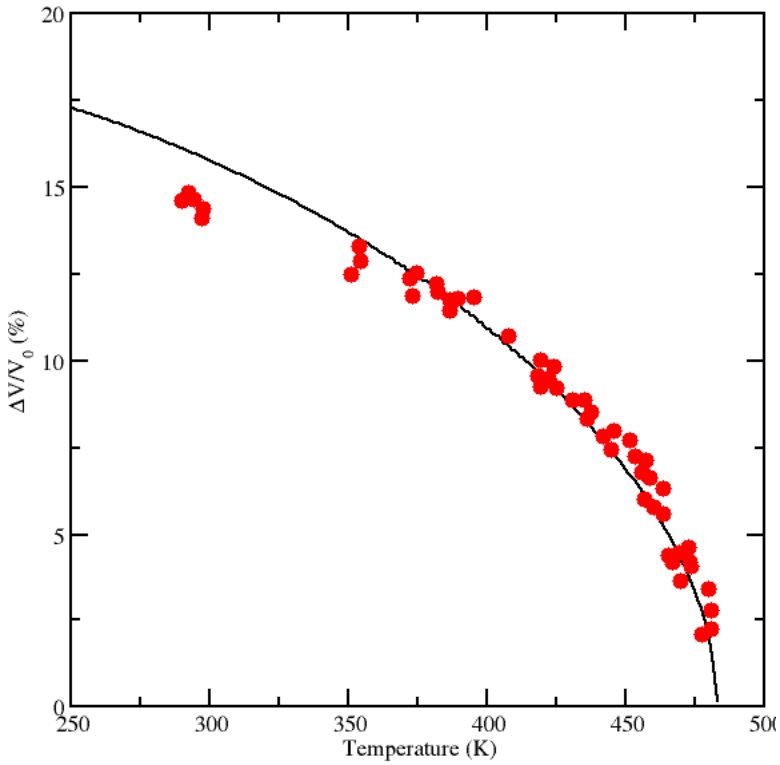
The equation of state is tabulated for computational efficiency

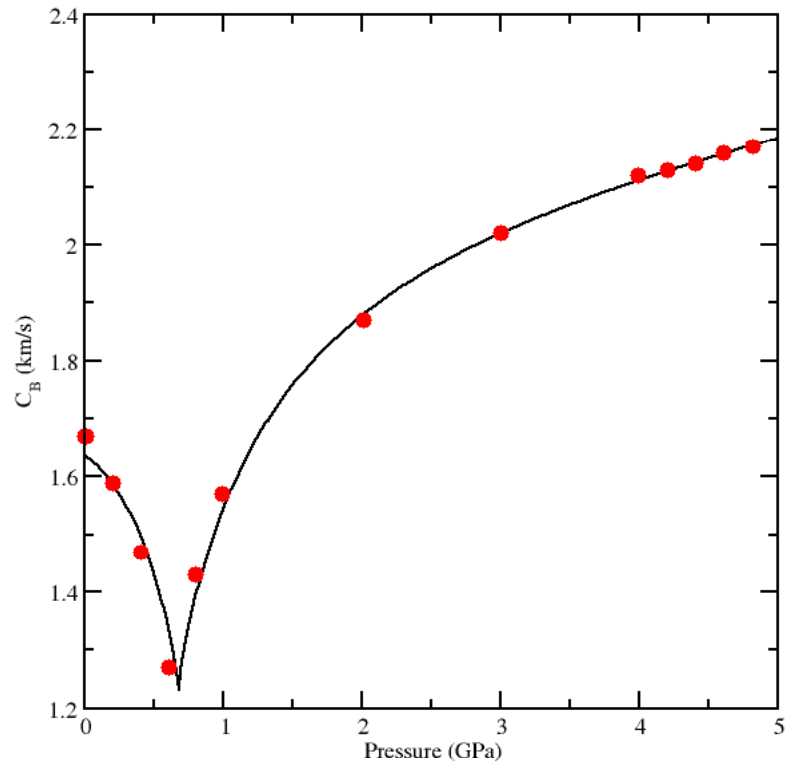
- **The Aptekar-Ponyatovsky model requires the finding of the composition of the solid solution for $\gamma-\alpha$ region of the phase diagram.**
  - This finding the roots for the composition can require a significant amount of computational time.
  - We thus tabulated the energies and pressures. We interpolate from the tables the appropriate variables at any given time step.
  - At a given time step we calculate analytically the sound velocity for the composition.
- **At the $\gamma-\alpha$ phase boundary a linear function of density with a slight slope was introduced**



The model predicts the static behavior of the γ−α phase boundary

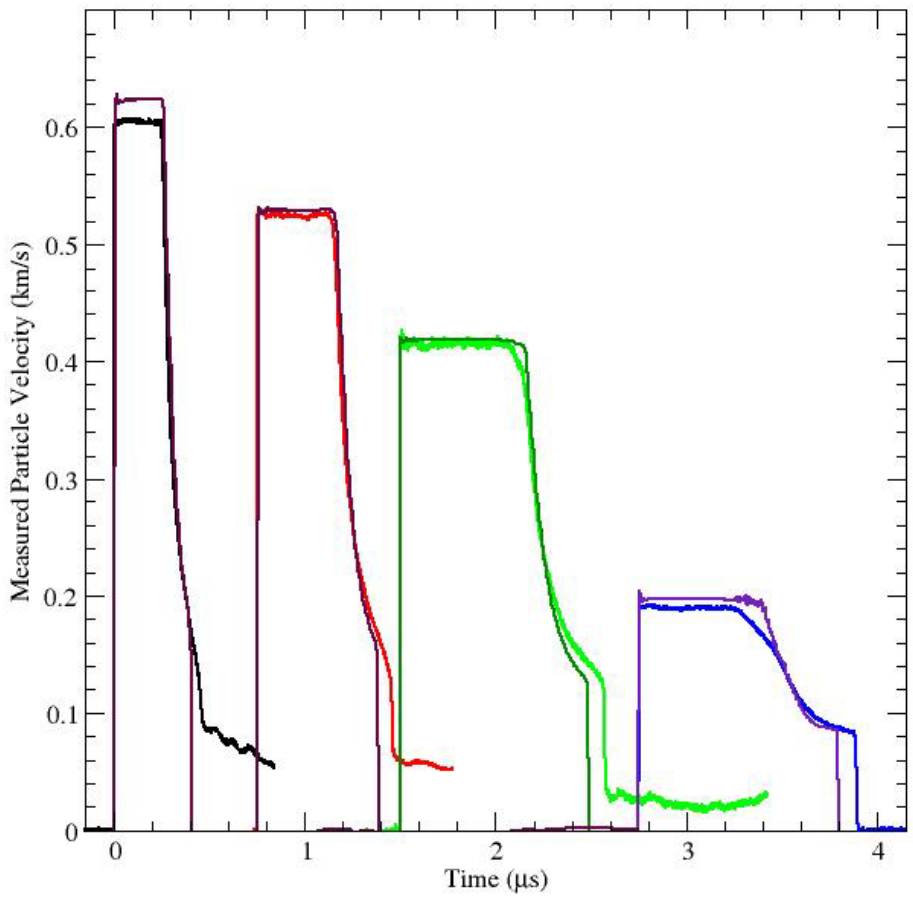
- The volume collapse and the bulk sound speed response of the material is captured by the model.



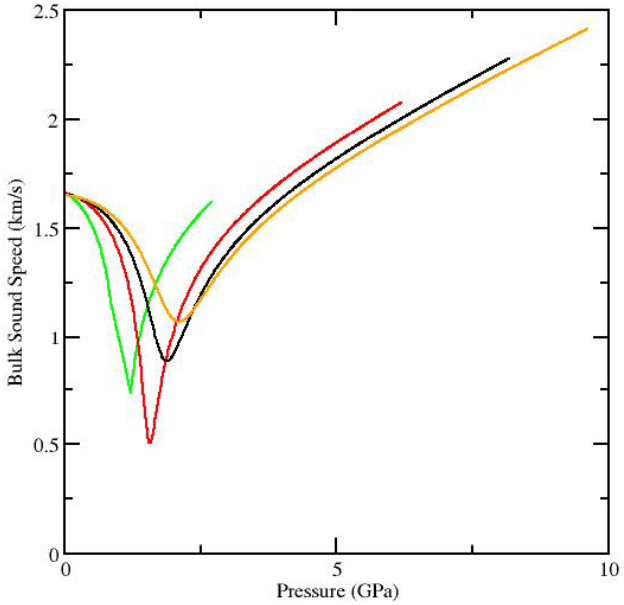


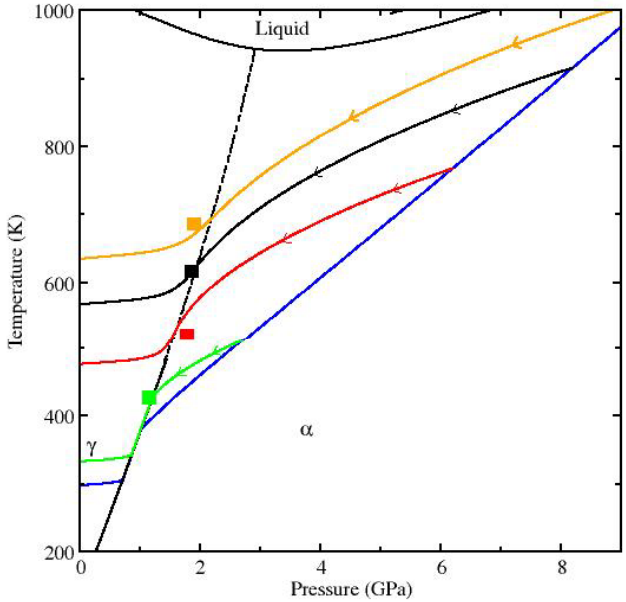
Front surface impact calculations compared with the corresponding experimental data

- **Simulations of the various experimental conditions were performed.**
  - Using a front surface impact configuration (Cerium impacting an aluminum coated LiF window) we calculated the experimental conditions of several experiments with a cerium impact velocity between 0.496 km/s to 1.29 km/s.
  - The model does not include anything to account for possible kinetics of the phase transition.
- **Model predicts the rarefaction shock.**
  - The stress state of the rarefaction shock is slightly over estimated in most cases.
  - Simulations include a simple elastic-plastic model for cerium.



Following the isentropic release of the model the temperature of the boundary is inferred.





Experiment	Observed Rarefaction Stress (GPa)	Calculated stress state (Gpa)	Calculated Temperature of Reversion (K)
56-06-25	1.15	1.22	428
69ss-06-15	1.78	1.57	523
69ss-09-04	1.86	1.89	617
69ss-09-10	1.89	2.11	687

Conclusions and Future Work

- **The multi-phase equation of state predicts the release behavior of cerium.**
- **A rarefaction shock is observed for those experiments above the solid-solid critical point.**
- **It may be necessary to include a different elastic-plastic model into the simulations to better show the release behavior of cerium.**
- **Future calculations of these particular experiments should include the foam backing the cerium.**
- **An adjustment of the phase boundary should be performed to better model the $\gamma-\alpha$ phase transition.**